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Abstract

A thermodynamic foundation using the concept of internal state variables is presented for the kinematic description of a viscoplastic material. Three different evolution equations for the back stress are considered. The first is that of classical, nonlinear, kinematic hardening. The other two include a contribution that is linear in stress rate. Choosing an appropriate change in variables can remove this stress rate dependence. As a result, one of these two models is shown to be equivalent to the classical, nonlinear, kinematic hardening model; while the other is a new model—one which seems to have favorable characteristics for representing ratchetting behavior. All three models are thermodynamically admissible.

Let us consider a complementary (Gibbs) free energy for the thermodynamic potential function, *i.e.*

$$\psi = \Psi[T, \sigma_{uv}, \beta_{uv}] \qquad , \qquad \beta_{ii} = 0 \, , \tag{1}$$

where square brackets $[\cdot]$ are used to denote 'function of'. The temperature T and stress σ_{ij} are external variables whose variations can, in principle, be controlled by an observer. However, the evolution of the internal state variable β_{ij}—associated with kinematic hardening—cannot be controlled by an observer; it is a material response. This variable must therefore evolve as a function of state. Furthermore, if this kinematic variable is to remain invariant under transformation to another kinematic variable, then its evolution will, in general, also depend upon the rates of change in the external variables [1]. For simplicity, let us consider the following equation for the evolution of internal state, *i.e.*

$$\dot{\beta}_{ij} = \dot{\chi}_{ij}[T, S_{uv}, \beta_{uv}] + (N/2H)\,\dot{S}_{ij} \, , \tag{2}$$

where $S_{ij} = \sigma_{ij} - {}^1\!/\!_3\, \sigma_{kk}\delta_{ij}$ is the deviatoric stress with δ_{ij} representing the Kronecker delta, and where N and H are material constants. In general, a term that is linear in $\dot{T}$ may also be introduced into (2) [2], but it is ignored in this paper for the purpose of simplification. Notice that β_{ij}, and therefore $\dot{\chi}_{ij}$, are deviatoric by definition. The function $\dot{\chi}_{ij}$ describes the irreversible contribution to the evolution of β_{ij}.

Given (1) and (2), one can derive [1, 2] relationships that govern the entropy,

$$S = \frac{-\partial\Psi}{\partial T} \, , \tag{3}$$

the strain,

$$\varepsilon_{ij} = \frac{-\partial\Psi}{\partial\sigma_{ij}} - \frac{N}{2H}\frac{\partial\Psi}{\partial\beta_{ij}} + \varepsilon^p_{ij} \qquad , \qquad \varepsilon^p_{ii} = 0 \, , \tag{4}$$

and the intrinsic dissipation,

$$\sigma_{ij}\dot{\varepsilon}^p_{ij} - \frac{\partial\Psi}{\partial\beta_{ij}}\,\dot{\chi}_{ij} \geq 0 \, , \tag{5}$$

where ε^p_{ij} is the plastic strain, which is deviatoric. It evolves according to a separate evolution equation (13).

If we assume that the complementary free energy (1) is given by

$$\begin{aligned} \Psi \;=\; & \overbrace{\frac{-1}{4\mu}\,S_{ij}S_{ij} - \frac{1}{18\kappa}\,\sigma_{ii}\sigma_{jj} - \alpha\,\Delta T\,\sigma_{ii} - S_0\Delta T - C\left\{T - T_0\left(1 + \ln\left[\frac{T}{T_0}\right]\right)\right\}}^{\text{thermoelastic contribution}} + \\ + \; & \underbrace{H\beta_{ij}\beta_{ij} + N\left(\frac{N}{4H}\,S_{ij}S_{ij} - \beta_{ij}S_{ij} + \Lambda[S_{uv},\beta_{uv}]\right)}_{\text{viscoplastic contribution}} \, , \end{aligned} \tag{6}$$

then we obtain—from (3) and (4)—the constitutive equations for an isotropic Hookean material ; they are:

$$\Delta S = \alpha\,\sigma_{ii} + (C/T)\Delta T \, , \tag{7}$$

$$\sigma_{ii} = 3\kappa\left(\varepsilon_{ii} - \alpha\,\Delta T\,\delta_{ii}\right) \, , \tag{8}$$

and

$$S_{ij} = 2\mu\left(E_{ij} - \varepsilon^p_{ij}\right) \, , \tag{9}$$

provided that

$$\frac{\partial\Lambda}{\partial S_{ij}} = \frac{-N}{2H}\frac{\partial\Lambda}{\partial\beta_{ij}} \, . \tag{10}$$

Here μ and κ are the elastic shear and bulk moduli, α is the coefficient of thermal expansion, C is the specific heat, S_0 and T_0 are the initial values of entropy and temperature with $\Delta S = S - S_0$ and $\Delta T = T - T_0$, and $E_{ij} = \varepsilon_{ij} - {}^1\!/_3\,\varepsilon_{kk}\delta_{ij}$ is the deviatoric strain. The first three terms in the viscoplastic contribution to Ψ are introduced to remove unwanted cross products that would otherwise appear in (9) because of (4) [2]. One also obtains

$$\frac{\partial\Psi}{\partial\beta_{ij}} = 2H\left(\beta_{ij} - \frac{N}{2H}S_{ij} - \frac{\partial\Lambda}{\partial S_{ij}}\right) = 2H\left(\chi_{ij} - \frac{\partial\Lambda}{\partial S_{ij}}\right) \, , \tag{11}$$

which defines the thermodynamic force conjugate to β_{ij}. As a consequence, (5) becomes

$$\sigma_{ij}\dot{\varepsilon}^p_{ij} - 2H\left(\chi_{ij} - \frac{\partial\Lambda}{\partial S_{ij}}\right)\dot{\chi}_{ij} \geq 0 \, , \tag{12}$$

which describes the intrinsic dissipation properties of our material. The function Λ, which is constrained by (10), is introduced into Ψ to affect the intrinsic dissipation (12); its form is model dependent.

For the evolution of plastic strain, we shall consider that

$$\dot{\varepsilon}^p_{ij} = 1/2 \, \| \dot{\boldsymbol{\varepsilon}}^p \| \, \frac{S_{ij} - B_{ij}}{\| \boldsymbol{S} - \boldsymbol{B} \|} \, , \tag{13}$$

where the back stress,

$$B_{ij} = 2H\beta_{ij} = 2H\chi_{ij} + NS_{ij} \, , \tag{14}$$

accounts for kinematic behavior, with $H > 0$ being its modulus and $0 \leq N < 1$. The norms used are defined by $\| \boldsymbol{I} \| = \sqrt{1/2 \, I_{ij} I_{ij}}$ where I_{ij} is any deviatoric stress-like quantity, and by $\| \boldsymbol{J} \| = \sqrt{2 J_{ij} J_{ij}}$ where J_{ij} is any deviatoric strain-like quantity. These von Mises norms are scaled for shear.

1 Model I

The classical, nonlinear, kinematic hardening model [3, 4] has an evolution of internal state described by

$$\dot{\chi}_{ij} = \dot{\varepsilon}^p_{ij} - \frac{H\chi_{ij}}{L} \, \| \dot{\boldsymbol{\varepsilon}}^p \| \, , \tag{15}$$

where L is the limiting state for the back stress B_{ij}. There is no stress rate term in the evolution of β_{ij} for this model, *i.e.* $N = 0$ in (2), and consequently

$$\dot{B}_{ij} = 2H \left(\dot{\varepsilon}^p_{ij} - \frac{B_{ij}}{2L} \, \| \dot{\boldsymbol{\varepsilon}}^p \| \right) \tag{16}$$

describes its evolution for the back stress. Because $N = 0$, the last three terms in the complementary free energy (6) do not contribute to the dissipation in this model; its intrinsic dissipation (12) is therefore given by

$$\left(\| \boldsymbol{S} - \boldsymbol{B} \| + \frac{\| \boldsymbol{B} \|^2}{L} \right) \| \dot{\boldsymbol{\varepsilon}}^p \| \geq 0 \, , \tag{17}$$

and it is always satisfied. Hence, Model I is thermodynamically admissible.

2 Model II

This model uses the same description for the irreversible evolution of internal state that Model I uses, *viz.* (15). In addition, it assumes that $0 < N < 1$, which introduces a reversible attribute to the evolution of internal state. As a result,

$$\dot{B}_{ij} = 2H \left(\dot{\varepsilon}^p_{ij} - \frac{B_{ij} - NS_{ij}}{2L} \, \| \dot{\boldsymbol{\varepsilon}}^p \| \right) + N\dot{S}_{ij} \tag{18}$$

describes this model's evolution for the back stress. Model II reduces to Model I when $N = 0$.

As Lubliner [1] discussed in his paper, one can always (in principle) transform from an internal state variable whose evolution contains terms that are linear in the external variable rates, to another internal state variable where there are no external variable rates present in the evolution equation. This is accomplished in our case by considering the linear transformation

$$X_{ij} = \frac{2H}{1 - N} \, \chi_{ij} = 2H' \chi_{ij} \, , \tag{19}$$

where the variable X_{ij} is a back stress, but different from B_{ij}, with $H' = H/(1-N)$ as its associated hardening modulus. This transformation enables the flow law (13) to be rewritten in an equivalent form as

$$\dot{\varepsilon}^{p}_{ij} = 1/2\, \|\dot{\boldsymbol{\varepsilon}}^{p}\| \, \frac{S_{ij} - X_{ij}}{\|\boldsymbol{S} - \boldsymbol{X}\|} \, . \tag{20}$$

Likewise, it allows the evolution equation for back stress (18) to be rewritten in the equivalent form

$$\dot{X}_{ij} = 2H' \left(\dot{\varepsilon}^{p}_{ij} - \frac{X_{ij}}{2L'} \, \|\dot{\boldsymbol{\varepsilon}}^{p}\| \right) \, , \tag{21}$$

where $L' = L/(1-N)$ is the limiting state for the back stress X_{ij}. Upon comparing (20) and (21) with (13) and (16), one observes that they are identical in mathematical structure, but with different values for their constants. These differences lead to differences in the intrinsic dissipation properties of the material [2].

From the perspective of material science [5], the physically correct, internal, state variable has an evolution equation with no $\dot{S}_{ij}$ or $\dot{T}$ dependence. This coincides with the experimental observation that an instantaneous change in either stress or temperature does not produce an instantaneous change in a material's internal structure, *i.e.* its dislocation structure. Consequently, the back stress X_{ij} is the physically correct back stress for Model II, and it is referred to as the physical back stress. (The back stress B_{ij} is the physical back stress of Model I.)

A description of Model II's dissipation response requires knowledge of its material function Λ, which is found in the expression for the complementary free energy (6). This function is evaluated by combining (12), (14), (15), (19), and (20), and then using Λ to cancel out those terms in the dissipation inequality that can become negative valued. This process leads to the differential equation

$$\frac{\partial \Lambda}{\partial S_{ij}} = \frac{N}{1-N} \left(\frac{N}{2H} \, S_{ij} - \beta_{ij} \right) \, , \tag{22}$$

which is the simplest of several possible solutions. This equation can be integrated, in conjunction with the constraint given in (10), to produce

$$\Lambda = \frac{N}{1-N} \left(\frac{N}{4H} \, S_{ij}S_{ij} - \beta_{ij}S_{ij} + \frac{H}{N} \, \beta_{ij}\beta_{ij} \right) \, , \tag{23}$$

which when substituted into (6) defines Ψ for Model II; it is the basic constitutive equation of this particular model. It follows then that the intrinsic dissipation (12) for Model II is given by the inequality

$$\left(\|\boldsymbol{S} - \boldsymbol{X}\| + \frac{\|\boldsymbol{X}\|^2}{L'} \right) \|\dot{\boldsymbol{\varepsilon}}^{p}\| \geq 0 \, , \tag{24}$$

and it is always satisfied. Hence, Model II is thermodynamically admissible. Notice the similarity between (17) and (24).

3 Model III

This model considers the irreversible evolution of internal state to be described by

$$\dot{\chi}_{ij} = \dot{\varepsilon}^{p}_{ij} - \frac{H\beta_{ij}}{L} \, \|\dot{\boldsymbol{\varepsilon}}^{p}\| \, , \tag{25}$$

which differs from (15) by the exchange of χ_{ij} with β_{ij} in the dynamic recovery term. Like Model II, this model takes $0 < N < 1$, and therefore

$$\dot{B}_{ij} = 2H\left(\dot{\varepsilon}^p_{ij} - \frac{B_{ij}}{2L}\,\|\dot{\boldsymbol{\varepsilon}}^p\|\right) + N\dot{S}_{ij} \tag{26}$$

describes the evolution for the back stress B_{ij}. Equation 26 was first proposed by Ramaswamy *et al.* [6]. Notice that the only difference between (16) and (26) for Models I and III is the presence of the term $N\dot{S}_{ij}$ found in (26). Model III reduces to Model I when $N = 0$.

Using the same linear transformation that was used in Model II, *i.e.* (19), one determines that Model III has the same transformed flow law (20) as Model II, but it has a different evolution equation for the physical back stress X_{ij}, *viz.*

$$\dot{X}_{ij} = \frac{2H}{1-N}\left(\dot{\varepsilon}^p_{ij} - \frac{(1-N)X_{ij} + NS_{ij}}{2L}\,\|\dot{\boldsymbol{\varepsilon}}^p\|\right) . \tag{27}$$

To the best of our knowledge, this ia a new expression for the evolution of the physical back stress. Here N proportions the dynamic recovery between the physical back stress X_{ij} and the applied stress S_{ij}.

We set out to derive the dissipation response of Model III as we did for Model II. We begin by considering a decomposition

$$\Lambda = \Lambda_1 + \Lambda_2 \, , \tag{28}$$

where Λ_1 is taken to be given by (23), *i.e.* Λ_1 is the Λ of Model II. The remaining function is evaluated by combining (12), (14), (19), (20), and (25), and then using Λ_2 to cancel out those remaining terms in the dissipation inequality that can become negative valued. Because of the constraint equation (10), one obtains two partial differential equations, *viz.*

$$\frac{\partial\Lambda_2}{\partial S_{ij}} = \frac{N}{2L(1-N)}\,S_{k\ell}\beta_{k\ell}\left(\frac{S_{ij} - 2H\beta_{ij}}{\|\boldsymbol{S} - 2H\boldsymbol{\beta}\|} - \frac{H\beta_{ij}}{L}\right)^{-1} , \tag{29}$$

$$\frac{\partial\Lambda_2}{\partial \beta_{ij}} = \frac{-H}{L(1-N)}\,S_{k\ell}\beta_{k\ell}\left(\frac{S_{ij} - 2H\beta_{ij}}{\|\boldsymbol{S} - 2H\boldsymbol{\beta}\|} - \frac{H\beta_{ij}}{L}\right)^{-1} , \tag{30}$$

which when integrated will lead to the complementary free energy Ψ for Model III, *i.e.* its fundamental constitutive equation. We have not integrated these equations. For our purpose, it is sufficient to know only that Λ exists. The intrinsic dissipation (12) for Model III is therefore given by the inequality

$$\left(\|\boldsymbol{S} - \boldsymbol{X}\| + \frac{\|\boldsymbol{B}\|^2}{L(1-N)}\right)\|\dot{\varepsilon}^p\| \geq 0 \, , \tag{31}$$

and it is always satisfied. Hence, Model III is also thermodynamically admissible.

A preliminary study of these three models [7] indicates that Model III may be able to predict realistic ratchetting behavior; whereas, Model I (and therefore Model II) is known to overpredict ratchetting behavior [8]. Continued research is required to better understand the predictive capabilities of Model III.

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16. Abstract

A thermodynamic foundation using the concept of internal state variables is presented for the kinematic description of a viscoplastic material. Three different evolution equations for the back stress are considered. The first is that of classical, nonlinear, kinematic hardening. The other two include a contribution that is linear in stress rate. Choosing an appropriate change in variables can remove this stress rate dependence. As a result, one of these two models is shown to be equivalent to the classical, nonlinear, kinematic hardening model; while the other is a new model—one which seems to have favorable characteristics for representing ratchetting behavior. All three models are thermodynamically admissible.

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